

Carbonic acid, 2-ethylhexyl octadecyl ester

Inchi: InChI=1S/C27H54O3/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-29-27(28)30
InchiKey: RIPSNWHZATWWAQ-UHFFFAOYSA-N
Formula: C27H54O3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 426.72

Physical Properties

Property code	Value	Unit	Source
gf	-164.90	kJ/mol	Joback Method
hf	-982.91	kJ/mol	Joback Method
hfus	66.14	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	9.618		Crippen Method
mvol	404.600	ml/mol	McGowan Method
pc	702.47	kPa	Joback Method
rinpol	2834.00		NIST Webbook
rinpol	2834.00		NIST Webbook
tb	915.43	K	Joback Method
tc	1126.32	K	Joback Method
tf	473.44	K	Joback Method
vc	1.583	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1385.29	J/molxK	915.43	Joback Method
cpg	1408.69	J/molxK	950.58	Joback Method
cpg	1430.46	J/molxK	985.73	Joback Method
cpg	1450.64	J/molxK	1020.88	Joback Method
cpg	1469.28	J/molxK	1056.02	Joback Method
cpg	1486.43	J/molxK	1091.17	Joback Method
cpg	1502.14	J/molxK	1126.32	Joback Method
dvisc	0.0005673	Paxs	473.44	Joback Method

dvisc	0.0002169	Paxs	547.11	Joback Method
dvisc	0.0001042	Paxs	620.77	Joback Method
dvisc	0.0000585	Paxs	694.43	Joback Method
dvisc	0.0000366	Paxs	768.10	Joback Method
dvisc	0.0000249	Paxs	841.76	Joback Method
dvisc	0.0000180	Paxs	915.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383145&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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